# organic compounds

## 4-Amino-3-(3-methoxybenzyl)-1H-1,2,4-triazole-5(4H)-thione

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In the title molecule, $C_{10}H_{12}N_4SO$, the triazole ring forms a dihedral angle of 73.0 (5)° with the benzene ring. The methoxy group is approximtely coplanar with the benzene ring with a C⋯C—O—$C_{methyl}$ torsion angle of 4.7 (3)°. In the crystal, N—H⋯S hydrogen bonds connect pairs of inversion-related molecules, which are in turn connected by N—H⋯N hydrogen bonds into chains of rings along [010]. Weak C—H⋯O hydrogen bonds connect these chains into a two-dimensional network parallel to ($\bar{1}$02).

## Related literature

For background to the chemistry of triazoles, see: Holla *et al.* (2001, 2006). For the biological activity of 1,2,4-triazole derivatives, see: Cansiz *et al.* (2001); Jones *et al.* (1965); Kane *et al.* (1988); Mullican *et al.* (1993). For related structures, see: Chen *et al.* (2007); Gao *et al.* (2011); Karczmarzyk *et al.* (2012). For standard bond-length data, see: Allen *et al.* (1987).
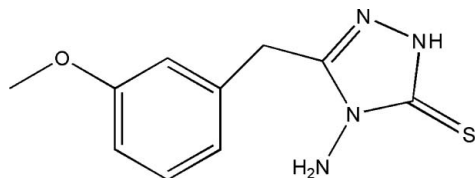


## Experimental

### Crystal data

| | |
|---|---|
| $C_{10}H_{12}N_4OS$ | $V = 1090.32$ (7) Å³ |
| $M_r = 236.30$ | $Z = 4$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a = 7.4580$ (3) Å | $\mu = 0.28$ mm$^{-1}$ |
| $b = 5.8006$ (2) Å | $T = 293$ K |
| $c = 25.2817$ (10) Å | $0.3 \times 0.2 \times 0.1$ mm |
| $\beta = 94.513$ (4)° | |

### Data collection

| | |
|---|---|
| Oxford Diffraction Xcalibur Sapphire3 diffractometer | 15190 measured reflections |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010) | 2130 independent reflections |
| | 1748 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.946$, $T_{max} = 1.000$ | $R_{int} = 0.042$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.088$ | |
| $S = 1.03$ | |
| 2130 reflections | $\Delta\rho_{max} = 0.19$ e Å$^{-3}$ |
| 154 parameters | $\Delta\rho_{min} = -0.24$ e Å$^{-3}$ |

### Table 1
Hydrogen-bond geometry (Å, °).

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C7—H7A⋯O1[i] | 0.97 | 2.46 | 3.308 (2) | 146 |
| N6—H62⋯N1[ii] | 0.90 (2) | 2.30 (2) | 3.190 (2) | 174 |
| N2—H2⋯S1[iii] | 0.86 | 2.60 | 3.377 (1) | 151 |

Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y + 1, z$; (iii) $-x + 2, -y + 2, -z + 2$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5605).

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# 4-Amino-3-(3-methoxybenzyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

## B. K. Sarojini, P. S. Manjula, Gurumurthy Hegde, Dalbir Kour, Sumati Anthal, Vivek K. Gupta and Rajni Kant

## Comment

The chemistry of triazoles has received considerable attention in recent years because of their versatility in the synthesis of many other heterocyclic compounds. 1,2,4-Triazole derivatives are well known for their different biological activities, therefore various 1,2,4-triazole derivatives and their N-bridged heterocyclic analogs have been extensively studied (Holla *et al.*, 2001; 2006). The derivatives of 1,2,4-triazole are known to exhibit anti-inflammatory (Mullican *et al.*, 1993), antiviral (Jones *et al.*, 1965), antimicrobial (Cansiz *et al.*, 2001), and antidepressant activity (Kane *et al.*, 1988). Hence, synthesis of the corresponding heterocyclic compounds could be of interest from the viewpoint of chemical reactivity and biological activity. In the title compound (Fig. 1), the bond lengths and angles have normal values (Allen *et al.*, 1987) and are comparable with closely related structures (Chen *et al.*, 2007; Karczmarzyk *et al.*, 2012; Gao *et al.*, 2011). The angles around atom C3 in the triazole ring deviate from the normal angles based on C$sp^2$ hybridization, giving bond angles of 102.72 (14)° and 130.12 (13)° for N2—C3—N4 and N2—C3—S1, respectively. The dihedral angle between the triazole ring (N1/N2/C3/N4/C5) and the benzene ring (C8—C13) is 73.0 (5)°. In the crystal, N—H⋯S hydrogen bonds connect pairs of inversion related molecules, which are in turn connected by N—H⋯N hydrogen bonds into chains of rings along [010]. In addition, weak C—H⋯O hydrogen bonds connect these chains into a two-dimensional network parallel to ($\bar{1}$02) (Fig. 2).

## Experimental

A well triturated mixture of 3-methoxyphenylacetic acid (0.83 g.0.05 mol) and thiocarbohydrazide (0.53 g. 0.05 mol) was fused in a round bottom flask for one hour on a oil bath at 413 K. It was cooled to room temperature and washed with sodium bicarbonate (5%) solution to remove unreacted acid and again washed with water. The dried compound was recrystallized from methanol to yield single crystals (mp. 417–419 K).

## Refinement

Atoms H61 and H62 attached to N6 were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically and were treated as riding on their parent C/N atoms, with C—H distances of 0.93–0.96 Å and N—H distance of 0.86 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C/N) or $U_{iso}$(H) = 1.5$U_{eq}$(C$_{methyl}$).

## Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).
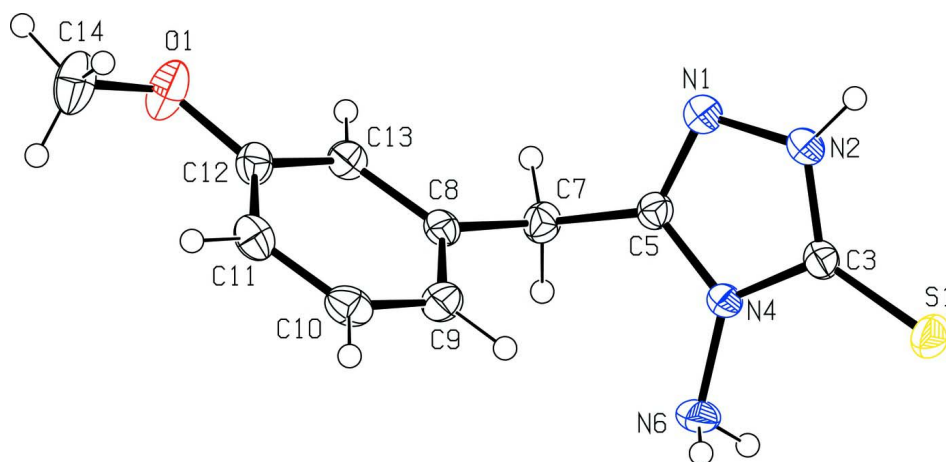
**Figure 1**

The molecular structure of the title compound with ellipsoids drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.
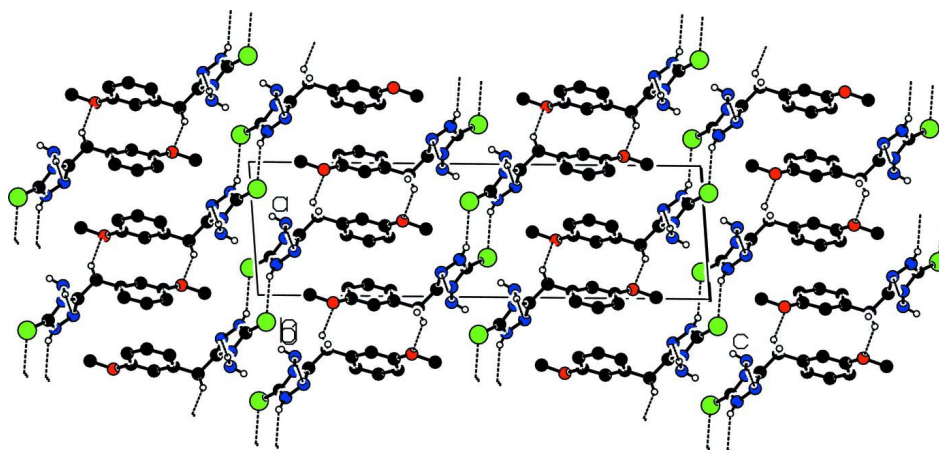


**Figure 2**

Part of the crystal structure with hydrogen bonds shown as dashed lines.

**4-Amino-3-(3-methoxybenzyl)-1*H*-1,2,4-triazole-5(4*H*)-thione**

*Crystal data*

| | |
|---|---|
| $C_{10}H_{12}N_4OS$ | $F(000) = 496$ |
| $M_r = 236.30$ | $D_x = 1.440$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 7374 reflections |
| $a = 7.4580$ (3) Å | $\theta = 3.5$–$29.0°$ |
| $b = 5.8006$ (2) Å | $\mu = 0.28$ mm$^{-1}$ |
| $c = 25.2817$ (10) Å | $T = 293$ K |
| $\beta = 94.513$ (4)° | Plate, white |
| $V = 1090.32$ (7) Å$^3$ | $0.3 \times 0.2 \times 0.1$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Sapphire3 diffractometer | 15190 measured reflections |
| Radiation source: fine-focus sealed tube | 2130 independent reflections |
| Graphite monochromator | 1748 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 16.1049 pixels mm$^{-1}$ | $R_{int} = 0.042$ |
| $\omega$ scans | $\theta_{max} = 26.0°$, $\theta_{min} = 3.5°$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010) | $h = -9 \rightarrow 9$ |
| | $k = -7 \rightarrow 7$ |
| $T_{min} = 0.946$, $T_{max} = 1.000$ | $l = -31 \rightarrow 31$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.088$ | |
| $S = 1.03$ | H atoms treated by a mixture of independent and constrained refinement |
| 2130 reflections | |
| 154 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.3289P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} = 0.002$ |
| | $\Delta\rho_{max} = 0.19$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.24$ e Å$^{-3}$ |

*Special details*

**Experimental**. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.79363 (6) | 1.26508 (8) | 1.014843 (19) | 0.03712 (16) |
| O1 | 0.4364 (2) | 0.7659 (2) | 0.66746 (5) | 0.0467 (4) |
| N1 | 0.6715 (2) | 0.7764 (2) | 0.91172 (6) | 0.0323 (4) |
| N2 | 0.77124 (19) | 0.8746 (2) | 0.95420 (6) | 0.0319 (4) |
| H2 | 0.8621 | 0.8077 | 0.9707 | 0.038* |
| C3 | 0.7134 (2) | 1.0833 (3) | 0.96726 (6) | 0.0254 (4) |
| N4 | 0.56824 (17) | 1.1164 (2) | 0.93177 (5) | 0.0239 (3) |
| C5 | 0.5471 (2) | 0.9287 (3) | 0.89877 (6) | 0.0246 (4) |
| N6 | 0.4558 (2) | 1.3106 (3) | 0.92853 (8) | 0.0360 (4) |
| C7 | 0.4041 (2) | 0.9044 (3) | 0.85492 (6) | 0.0284 (4) |
| H7A | 0.2994 | 0.9908 | 0.8639 | 0.034* |
| H7B | 0.3696 | 0.7434 | 0.8519 | 0.034* |
| C8 | 0.4584 (2) | 0.9870 (3) | 0.80138 (6) | 0.0249 (4) |

| | | | |
|---|---|---|---|
| C9 | 0.5382 (2) | 1.2018 (3) | 0.79529 (7) | 0.0322 (4) |
| H9 | 0.5617 | 1.2972 | 0.8246 | 0.039* |
| C10 | 0.5823 (2) | 1.2730 (3) | 0.74597 (8) | 0.0339 (4) |
| H10 | 0.6347 | 1.4170 | 0.7423 | 0.041* |
| C11 | 0.5501 (2) | 1.1344 (3) | 0.70177 (7) | 0.0328 (4) |
| H11 | 0.5805 | 1.1838 | 0.6686 | 0.039* |
| C12 | 0.4717 (2) | 0.9206 (3) | 0.70779 (7) | 0.0290 (4) |
| C13 | 0.4246 (2) | 0.8490 (3) | 0.75726 (7) | 0.0271 (4) |
| H13 | 0.3696 | 0.7064 | 0.7607 | 0.032* |
| C14 | 0.4954 (3) | 0.8208 (4) | 0.61719 (8) | 0.0492 (5) |
| H14A | 0.4348 | 0.9572 | 0.6037 | 0.074* |
| H14B | 0.4686 | 0.6950 | 0.5932 | 0.074* |
| H14C | 0.6228 | 0.8475 | 0.6205 | 0.074* |
| H62 | 0.524 (3) | 1.436 (4) | 0.9246 (8) | 0.049 (6)* |
| H61 | 0.403 (3) | 1.324 (4) | 0.9573 (10) | 0.065 (8)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0330 (3) | 0.0444 (3) | 0.0325 (3) | 0.0079 (2) | −0.00694 (19) | −0.0124 (2) |
| O1 | 0.0607 (9) | 0.0517 (8) | 0.0284 (7) | −0.0206 (7) | 0.0078 (6) | −0.0085 (6) |
| N1 | 0.0352 (8) | 0.0312 (8) | 0.0297 (9) | 0.0065 (6) | −0.0034 (7) | −0.0030 (6) |
| N2 | 0.0317 (8) | 0.0324 (8) | 0.0303 (8) | 0.0109 (6) | −0.0064 (7) | −0.0018 (6) |
| C3 | 0.0232 (8) | 0.0305 (9) | 0.0227 (9) | 0.0032 (7) | 0.0025 (7) | 0.0025 (7) |
| N4 | 0.0223 (7) | 0.0239 (7) | 0.0250 (7) | 0.0044 (5) | −0.0015 (6) | −0.0009 (6) |
| C5 | 0.0267 (8) | 0.0244 (8) | 0.0228 (9) | −0.0007 (7) | 0.0033 (7) | 0.0004 (6) |
| N6 | 0.0353 (9) | 0.0290 (9) | 0.0422 (11) | 0.0141 (7) | −0.0073 (8) | −0.0061 (7) |
| C7 | 0.0264 (9) | 0.0310 (9) | 0.0273 (9) | −0.0015 (7) | −0.0010 (7) | −0.0032 (7) |
| C8 | 0.0204 (8) | 0.0265 (8) | 0.0272 (9) | 0.0033 (6) | −0.0028 (7) | 0.0003 (7) |
| C9 | 0.0355 (10) | 0.0263 (9) | 0.0341 (10) | −0.0017 (7) | −0.0023 (8) | −0.0043 (7) |
| C10 | 0.0326 (10) | 0.0238 (9) | 0.0450 (11) | −0.0031 (7) | 0.0003 (8) | 0.0055 (8) |
| C11 | 0.0311 (9) | 0.0363 (10) | 0.0310 (10) | −0.0006 (8) | 0.0016 (8) | 0.0079 (8) |
| C12 | 0.0261 (9) | 0.0335 (9) | 0.0267 (9) | −0.0010 (7) | −0.0012 (7) | −0.0008 (7) |
| C13 | 0.0256 (9) | 0.0248 (8) | 0.0304 (10) | −0.0024 (7) | −0.0004 (7) | 0.0008 (7) |
| C14 | 0.0469 (13) | 0.0726 (15) | 0.0287 (11) | −0.0096 (11) | 0.0073 (9) | −0.0059 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C3 | 1.6745 (17) | C7—H7B | 0.9700 |
| O1—C12 | 1.368 (2) | C8—C13 | 1.380 (2) |
| O1—C14 | 1.414 (2) | C8—C9 | 1.395 (2) |
| N1—C5 | 1.304 (2) | C9—C10 | 1.377 (3) |
| N1—N2 | 1.381 (2) | C9—H9 | 0.9300 |
| N2—C3 | 1.335 (2) | C10—C11 | 1.382 (3) |
| N2—H2 | 0.8600 | C10—H10 | 0.9300 |
| C3—N4 | 1.364 (2) | C11—C12 | 1.384 (2) |
| N4—C5 | 1.373 (2) | C11—H11 | 0.9300 |
| N4—N6 | 1.4029 (19) | C12—C13 | 1.389 (2) |
| C5—C7 | 1.483 (2) | C13—H13 | 0.9300 |
| N6—H62 | 0.90 (2) | C14—H14A | 0.9600 |

| | | | |
|---|---|---|---|
| N6—H61 | 0.86 (3) | C14—H14B | 0.9600 |
| C7—C8 | 1.521 (2) | C14—H14C | 0.9600 |
| C7—H7A | 0.9700 | | |
| | | | |
| C12—O1—C14 | 117.84 (15) | C13—C8—C7 | 119.48 (15) |
| C5—N1—N2 | 104.16 (13) | C9—C8—C7 | 121.71 (15) |
| C3—N2—N1 | 113.69 (14) | C10—C9—C8 | 120.12 (16) |
| C3—N2—H2 | 123.2 | C10—C9—H9 | 119.9 |
| N1—N2—H2 | 123.2 | C8—C9—H9 | 119.9 |
| N2—C3—N4 | 102.72 (14) | C9—C10—C11 | 121.26 (16) |
| N2—C3—S1 | 130.12 (13) | C9—C10—H10 | 119.4 |
| N4—C3—S1 | 127.17 (12) | C11—C10—H10 | 119.4 |
| C3—N4—C5 | 109.59 (13) | C10—C11—C12 | 118.69 (17) |
| C3—N4—N6 | 126.24 (14) | C10—C11—H11 | 120.7 |
| C5—N4—N6 | 124.17 (14) | C12—C11—H11 | 120.7 |
| N1—C5—N4 | 109.83 (15) | O1—C12—C11 | 124.32 (16) |
| N1—C5—C7 | 125.34 (15) | O1—C12—C13 | 115.29 (15) |
| N4—C5—C7 | 124.83 (14) | C11—C12—C13 | 120.39 (16) |
| N4—N6—H62 | 108.4 (14) | C8—C13—C12 | 120.74 (15) |
| N4—N6—H61 | 109.5 (17) | C8—C13—H13 | 119.6 |
| H62—N6—H61 | 109 (2) | C12—C13—H13 | 119.6 |
| C5—C7—C8 | 114.15 (14) | O1—C14—H14A | 109.5 |
| C5—C7—H7A | 108.7 | O1—C14—H14B | 109.5 |
| C8—C7—H7A | 108.7 | H14A—C14—H14B | 109.5 |
| C5—C7—H7B | 108.7 | O1—C14—H14C | 109.5 |
| C8—C7—H7B | 108.7 | H14A—C14—H14C | 109.5 |
| H7A—C7—H7B | 107.6 | H14B—C14—H14C | 109.5 |
| C13—C8—C9 | 118.79 (16) | | |
| | | | |
| C5—N1—N2—C3 | −0.81 (19) | C5—C7—C8—C13 | 132.14 (16) |
| N1—N2—C3—N4 | 1.00 (18) | C5—C7—C8—C9 | −49.4 (2) |
| N1—N2—C3—S1 | −179.11 (13) | C13—C8—C9—C10 | −0.1 (3) |
| N2—C3—N4—C5 | −0.80 (17) | C7—C8—C9—C10 | −178.66 (16) |
| S1—C3—N4—C5 | 179.30 (13) | C8—C9—C10—C11 | −0.4 (3) |
| N2—C3—N4—N6 | 179.29 (16) | C9—C10—C11—C12 | 0.1 (3) |
| S1—C3—N4—N6 | −0.6 (3) | C14—O1—C12—C11 | 4.7 (3) |
| N2—N1—C5—N4 | 0.25 (18) | C14—O1—C12—C13 | −174.70 (17) |
| N2—N1—C5—C7 | −179.94 (15) | C10—C11—C12—O1 | −178.59 (17) |
| C3—N4—C5—N1 | 0.36 (19) | C10—C11—C12—C13 | 0.8 (3) |
| N6—N4—C5—N1 | −179.74 (16) | C9—C8—C13—C12 | 1.0 (2) |
| C3—N4—C5—C7 | −179.46 (15) | C7—C8—C13—C12 | 179.59 (15) |
| N6—N4—C5—C7 | 0.4 (3) | O1—C12—C13—C8 | 178.05 (15) |
| N1—C5—C7—C8 | −87.4 (2) | C11—C12—C13—C8 | −1.4 (3) |
| N4—C5—C7—C8 | 92.39 (19) | | |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C7—H7*A*···O1[i] | 0.97 | 2.46 | 3.308 (2) | 146 |

| N6—H62⋯N1ⁱⁱ | 0.90 (2) | 2.30 (2) | 3.190 (2) | 174 |
|---|---|---|---|---|
| N2—H2⋯S1ⁱⁱⁱ | 0.86 | 2.60 | 3.377 (1) | 151 |

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2; (ii) *x*, *y*+1, *z*; (iii) −*x*+2, −*y*+2, −*z*+2.